Neutron Reflection Conditions for Magnetic Lattices and Symmetry Operations

SHIP student: Daniel Sun, Poolesville High School

Mentor: Qingzhen Huang, NCNR

Abstract

Materials with magnetic properties are more and more interesting in daily life. Neutron technique is one of the most useful methods for investigating magnetic structure and properties. We used simulation to model the 36 magnetic lattices and symmetry operations, and to analyze the magnetic structure factor for neutron diffraction. We conclude systematic absence of magnetic neutron diffraction for the magnetic lattice and symmetry operations. The reflection conditions for nuclear diffraction and magnetic diffraction are compared and discussed.

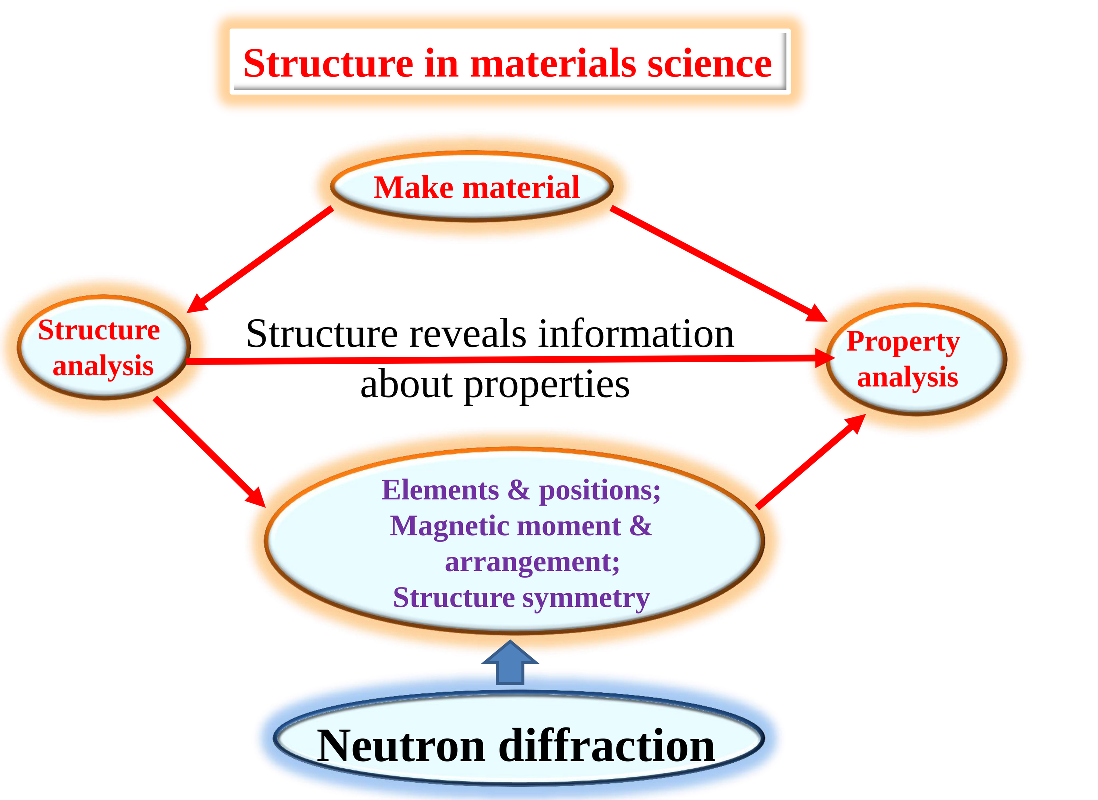


Fig 1. Relationship between structure and properties. When a material is made, we are expected to know the structure and properties, and to find the relationships. The structure analysis will help us modify the crystal structure and therefore to design a new structure and improve the properties. In materials with magnetic properties, neutron diffraction is one of the most useful techniques. One can use the neutron powder diffractometer to measure the diffraction intensities, as shown in Fig. 2.

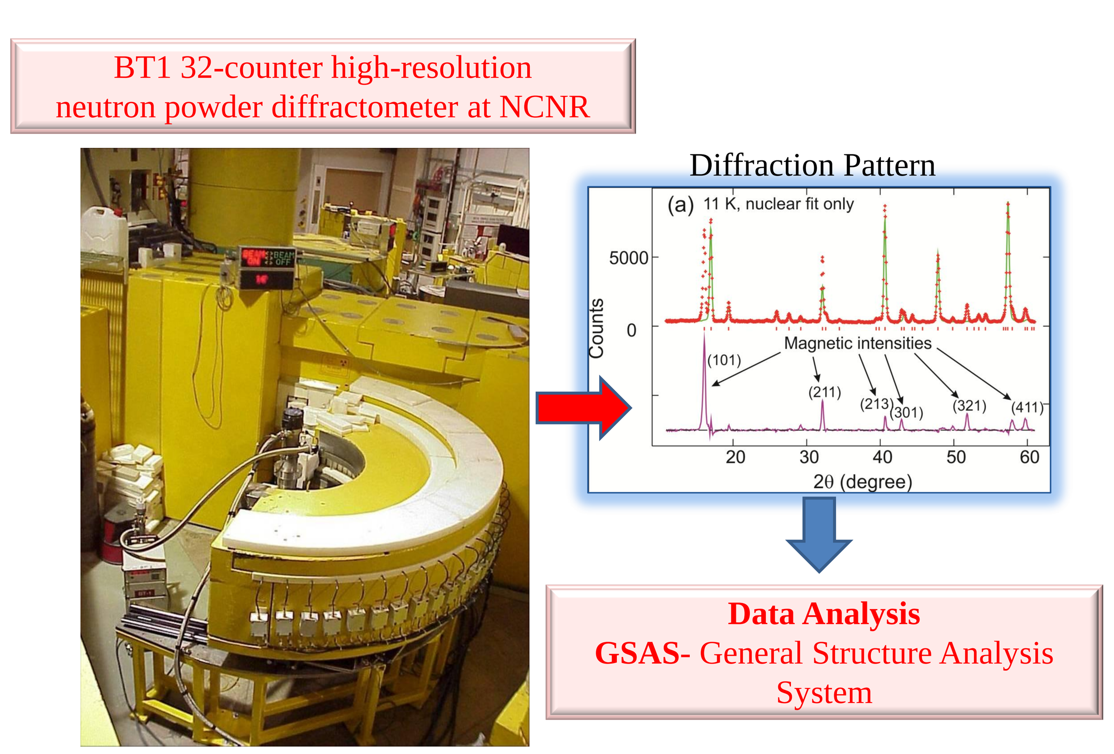


Fig 2. Neutron powder diffractometer at NCNR (left) and an example of a powder diffraction pattern (right up). The observed data (crosses), the calculated nuclear intensities (green solid line), and the magnetic diffraction intensities (bottom, solid line of the differences between observed and calculated intensities) are shown in the figure. Fit was performed by using a General Structure Analysis System (GSAS)* Program.

*Larson, A. C. & Von Dreele, A. C. Los Alamos National Laboratory Report No. LAUR086-748 (1990).

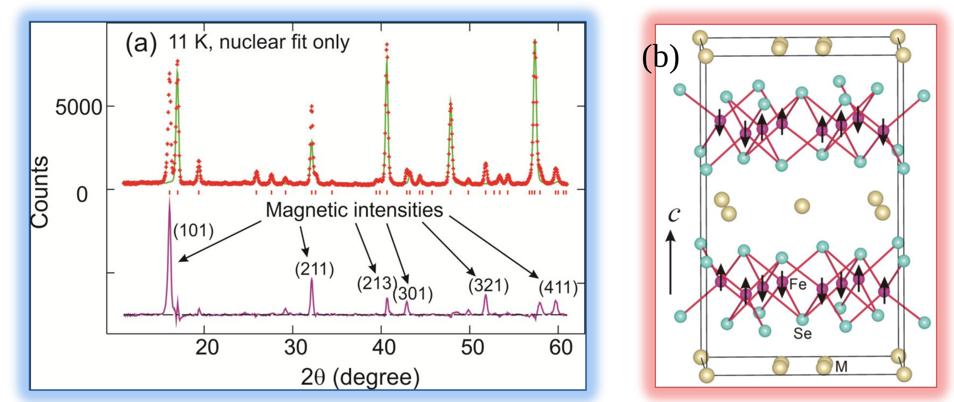


Fig 3. Neutron powder diffraction data and the magnetic structure of the material.

The neutron powder diffraction data contains crystal and magnetic structure information. For example, the diffraction pattern in figure 3a contains both crystal and magnetic structure information for a compound with the structure as shown in figure 3b. We can use the diffraction pattern to determine the crystal and magnetic structures.

1) Peak position: $2d\sin q = n\lambda$;

2) Nuclear diffraction intensities: $I_N = CM_T\,[(\gamma e^2)/(2mc^2)]^2\,|F_N|^2$;

3) Magnetic diffraction intensities: $I_M = CM_T\,A(\theta_B)\,[(\gamma e^2)/(2mc^2)]^2 \langle 1-(\tau\cdot M)^2\rangle |F_M|^2$.

where F is the structure factor in which contains all the structure information. The equation for F is:

$$F_{hkl} = \sum \mu f \exp(2\pi\iota\,(hM_x + kM_y + lM_z)) \qquad (1)$$

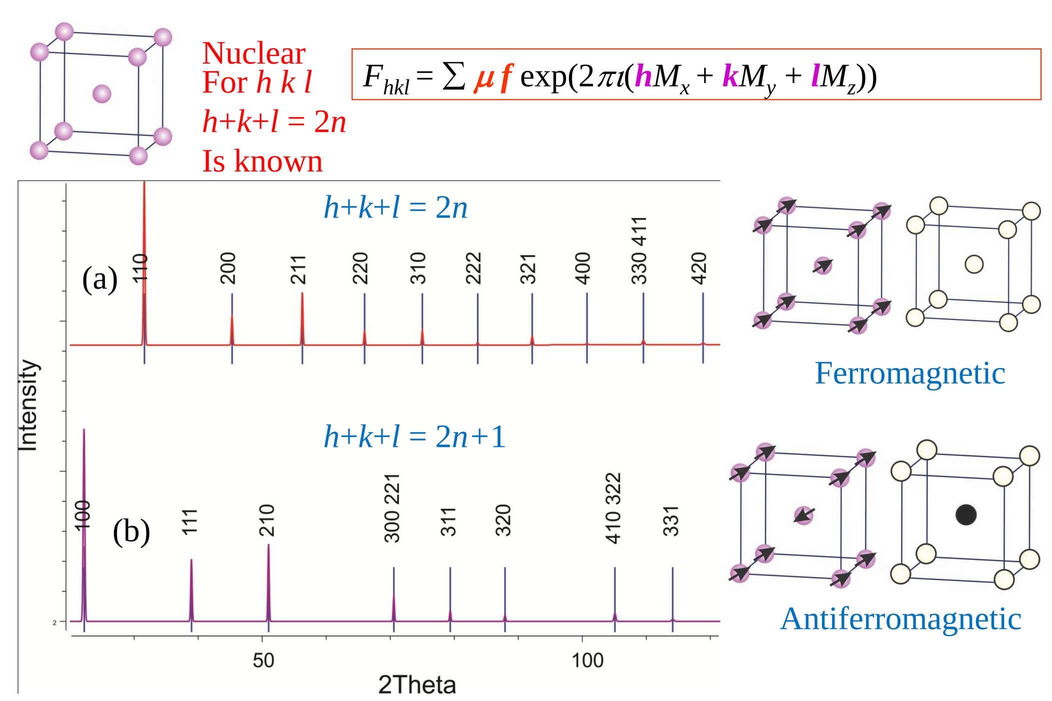
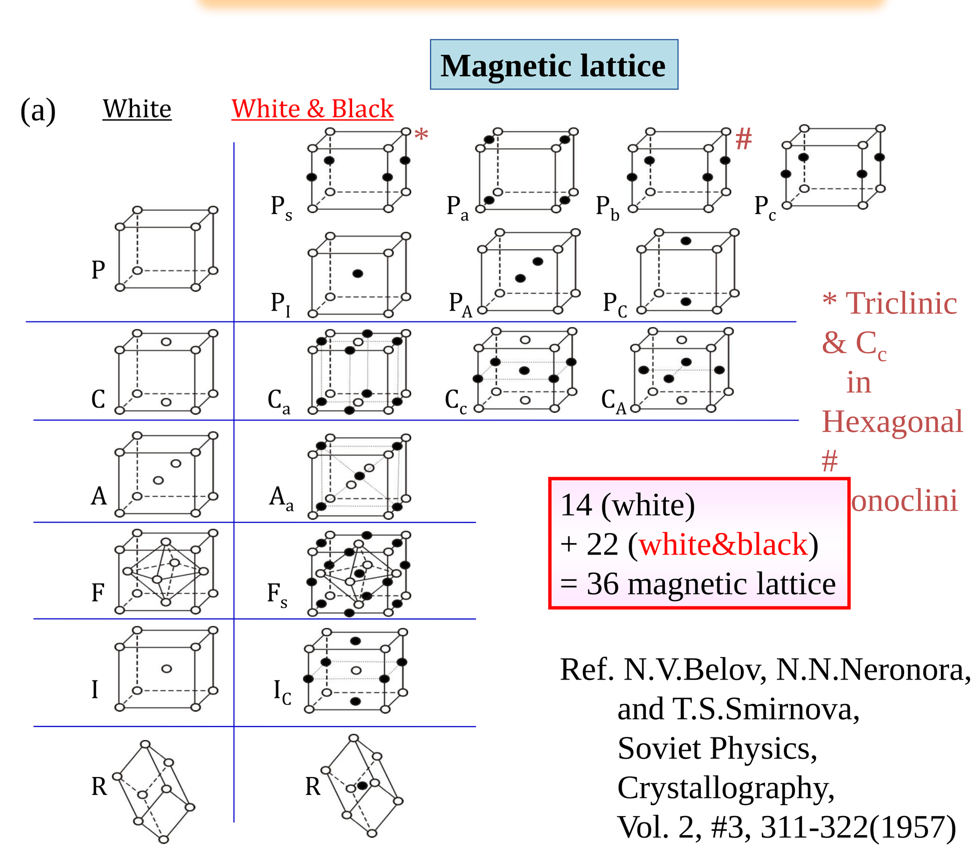


Fig 4. Reflection condition analysis. Different magnetic lattices give unique diffraction patterns. (a) calculated pattern for body-centered ferromagnetic lattice where only reflections having $h+k+l = 2n$ appear. (b) calculated pattern for body-centered antiferromagnetic lattice where only reflections having $h+k+l = 2n+1$ appear. These reflection conditions will help us find the magnetic lattice and symmetry operations, *i.e.* to determine the magnetic symmetry of space group.

36 black & white magnetic lattices



Ref. N.V.Belov, N.N.Neronora, and T.S.Smirnova, Soviet Physics, Crystallography, Vol. 2, #3, 311-322(1957)

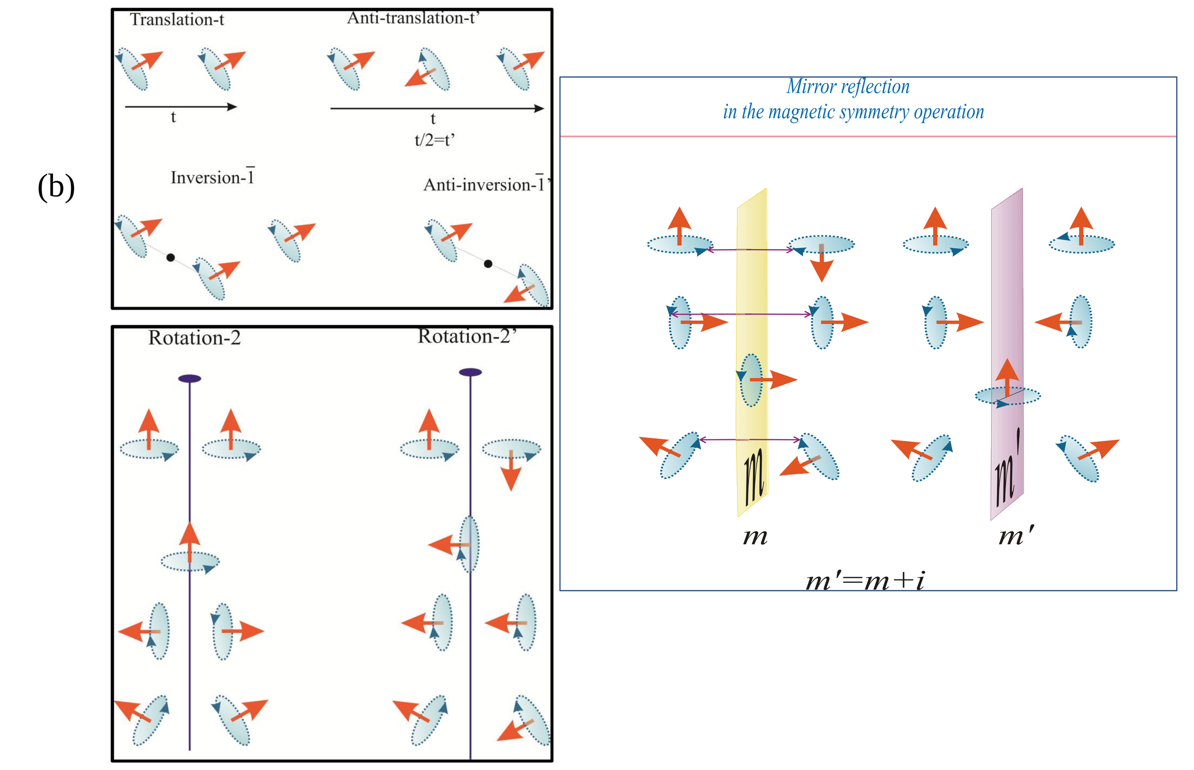


Fig 5. (a) the 36 magnetic black and white lattices. (b) Some of the magnetic symmetry operations.

The reflection conditions for the 36 magnetic lattices (Fig. 5a) and symmetry operations (Fig. 5b) were analyzed by calculating the structure factor for magnetic reflections using GSAS. As shown in Figure 6, the calculated F^2 (function (1)) as a function of Δx (a shift from the ideal position of the body-centered, in the left figure). If there are impurities in the crystal, the coordinates will not form symmetry exactly, so there must be a limit of what can be considered systematic absence.

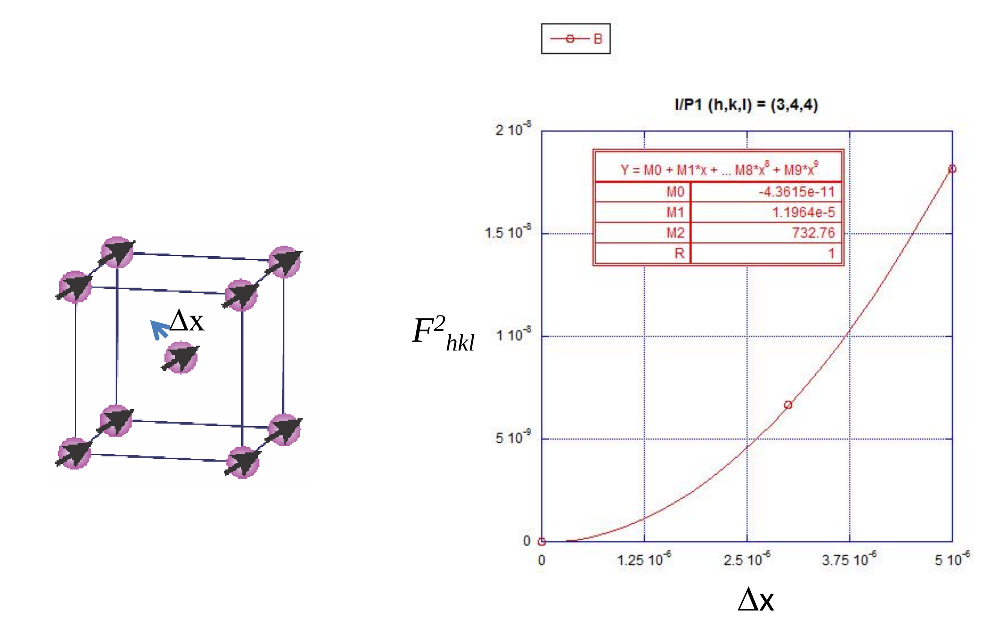


Fig. 6. Simulations were done using GSAS. This is the graph of the maximum structure factor as a function of Δx. The threshold of 10^{-8} is passed at approximately 3.7×10^{-6}.

Results of the magnetic reflection conditions

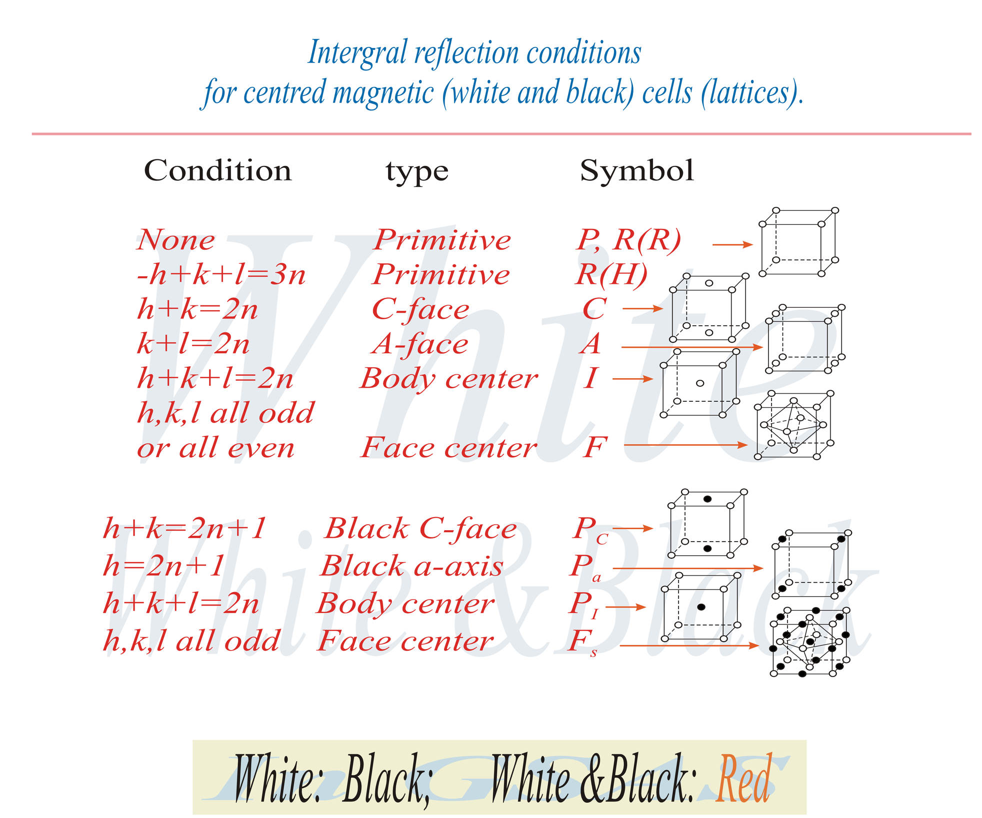


Fig 7. The reflection conditions for the lattice centering functions for white and black lattices.

Symmetry Operation	Nuclear Reflection Condition	Magnetic Reflection Condition*
a (*a*-glide)	$k + l = 2n$	None
b (*b*-glide)	$h + l = 2n$	None
c (*c*-glide)	$h + k = 2n$	None
2_1	$0k0$: $k = 2n$	$0k0$: $k = 2n + 1$
$2'_1$	--	$0k0$: $k = 2n$
4_i (i=1, 3)	$00l$: $l = 4n$	$00l$: $l = 2n+1$
$4'_i$ (i=1, 3)	--	$00l$: $l = 2n+1$
3_i (i = 1, 2)	$00l$: $l = 3n$	$00l$: $l \neq 3n$
6_i (i = 1, 5)	$00l$: $l = 6n$	$00l$: $l = 2n + 1 \neq 3n$

Fig 8. nuclear and magnetic reflection conditions for symmetry operations

In table, the prime " ' " is the operation of spin flip, which is not considered in nuclear diffraction, so there are no nuclear reflection conditions for these symmetry operations. This makes the magnetic reflection conditions for symmetry operations much more difficult. Since a ferromagnetic lattice has the same magnetic reflection conditions as nuclear reflection conditions, a magnetic moment in one direction will give an antiferromagnetic lattice, whereas a magnetic moment in a different direction will give a ferromagnetic lattice (as shown in Fig. 5b). The results listed are the ones which give antiferromagnetic lattices, since there is only one direction of magnetic moment which will give a ferromagnetic lattice for each symmetry operation.

Also, some of the magnetic symmetry operations do not have reflection conditions, most notably seen in the glide operations. I will do mathematical analysis of the F^2 formula to see why certain symmetry operations do not have magnetic reflection conditions.

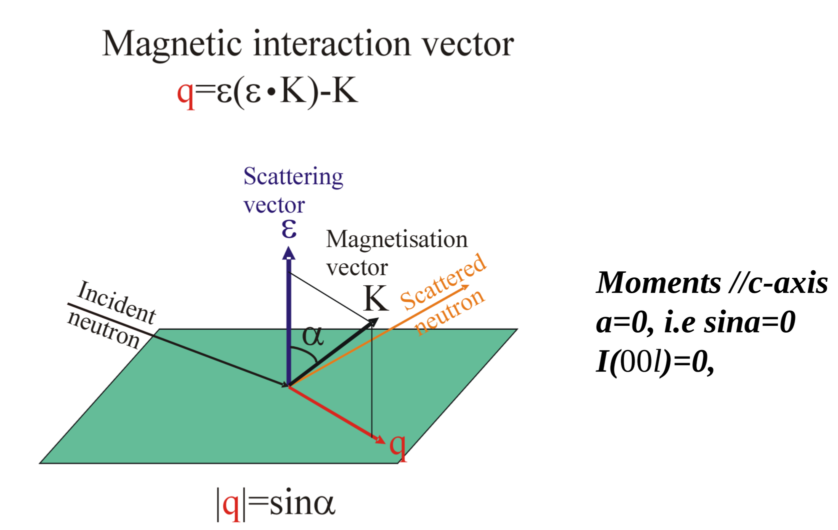


Fig 9. Definition of magnetic diffraction.

The magnetic interaction vector is defined q= ε(ε · K)-K. When **K** is parallel to **ε**, q will be 0. Therefore, the structure factor is measured as 0 when the scattered vector (*h*, *k*, *l*) is parallel to the magnetic moment. It is important to note the direction of the magnetic moment, because the scattering vector could be parallel to the magnetic moment and still meet reflection conditions. This can be seen in figure 3. The material in figure 3 has ferromagnetic body-centered lattice, because we have found that the observed reflections have condition of $h + k + l = 2n$, however, (0, 0, 2) is absent. it is because that the magnetic moment is parallel to the scattering vector of (002) .

Further plan

To analyze the magnetic reflection conditions

- Change in magnetic moment amplitude
- Change in magnetic moment orientation
- Confirm results by analyzing F^2 formula